



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:44 PM GMT

PDB ID : 2R00
Title : crystal structure of aspartate semialdehyde dehydrogenase II complexed with ASA from vibrio cholerae
Authors : Viola, R.E.; Liu, X.; Ohren, J.F.; Faehnle, C.R.
Deposited on : 2007-08-17
Resolution : 2.03 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

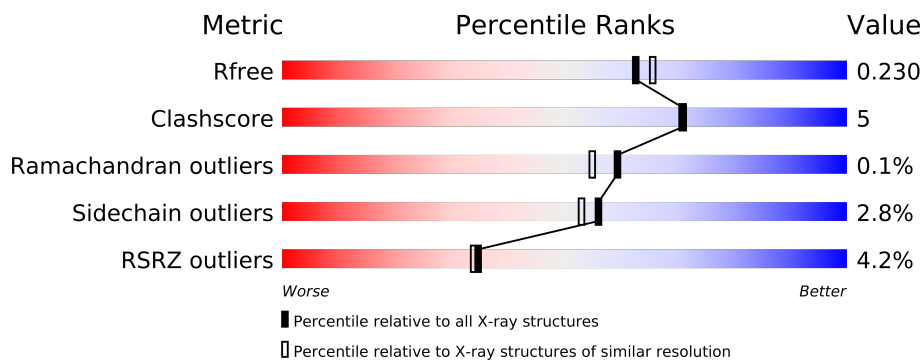
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.03 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	6003 (2.04-2.00)
Clashscore	79885	7467 (2.04-2.00)
Ramachandran outliers	78287	7370 (2.04-2.00)
Sidechain outliers	78261	7368 (2.04-2.00)
RSRZ outliers	66119	6006 (2.04-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	336	
1	B	336	
2	C	336	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	OEG	C	1	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 7992 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

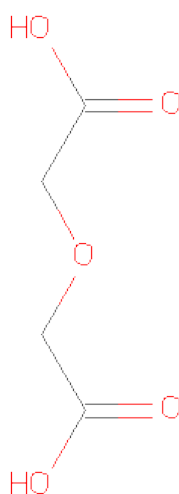
- Molecule 1 is a protein called Aspartate-semialdehydedehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	2	0
			2389	1510	409	460	10			
1	B	302	Total	C	N	O	S	0	0	0
			2370	1506	399	454	11			

- Molecule 2 is a protein called Aspartate-semialdehydedehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	336	Total	C	N	O	S	0	3	0
			2624	1658	446	509	11			

- Molecule 3 is 2,2'-OXYDIACETIC ACID (three-letter code: OEG) (formula: C₄H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			9	4	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	186	Total 186	O 186	0	0
4	B	177	Total 177	O 177	0	0
4	C	237	Total 237	O 237	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.38Å 84.68Å 114.98Å 90.00° 102.07° 90.00°	Depositor
Resolution (Å)	40.00 – 2.03 33.82 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.00-2.03) 99.4 (33.82-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.191 , 0.232 0.191 , 0.230	Depositor DCC
R_{free} test set	3747 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 74272 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7992	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OEG, HTI

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.81	2/2448 (0.1%)	0.74	2/3328 (0.1%)
1	B	0.46	0/2419	0.57	0/3291
2	C	0.52	0/2667	0.61	1/3626 (0.0%)
All	All	0.61	2/7534 (0.0%)	0.64	3/10245 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	LYS	C-N	28.50	1.99	1.34
1	A	213	LYS	C-O	15.73	1.53	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	LYS	O-C-N	-21.29	88.64	122.70
1	A	213	LYS	CA-C-O	14.20	149.92	120.10
2	C	311	LEU	CA-CB-CG	6.22	129.61	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2389	0	2305	30	0
1	B	2370	0	2287	15	0
2	C	2624	0	2541	23	0
3	C	9	0	4	4	0
4	A	186	0	0	5	0
4	B	177	0	0	2	0
4	C	237	0	0	10	0
All	All	7992	0	7137	66	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (66) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:213:LYS:C	1:A:214:GLU:N	1.99	1.14
2:C:97:ASN:HD21	3:C:1:OEG:H2	1.24	0.99
2:C:97:ASN:ND2	3:C:1:OEG:H2	1.86	0.90
1:A:78[A]:GLU:OE2	4:A:515:HOH:O	1.98	0.81
3:C:1:OEG:O5	4:C:537:HOH:O	1.99	0.80
1:A:162:VAL:HA	1:A:239:ARG:HG2	1.64	0.79
1:A:135:THR:HG22	1:A:139:LEU:HD12	1.68	0.75
1:A:251:HIS:HE1	1:A:302:ASP:OD2	1.80	0.63
2:C:104:ASP:OD1	4:C:564:HOH:O	2.15	0.63
1:A:335:ARG:HD2	1:A:336:ASP:OD1	1.99	0.62
1:B:133:CYS:HB2	1:B:318:VAL:HG22	1.81	0.61
2:C:130:ASN:ND2	2:C:325:ASN:HD22	2.00	0.59
1:B:215:GLU:O	1:B:235:PRO:HG2	2.03	0.58
1:B:213:LYS:NZ	4:B:647:HOH:O	2.36	0.58
1:A:130:ASN:ND2	1:A:325:ASN:HD22	2.01	0.57
2:C:269:GLN:HG2	4:C:570:HOH:O	2.04	0.57
1:B:188:THR:HG23	1:B:191:PHE:H	1.70	0.57
1:A:125:ARG:NH1	4:A:413:HOH:O	2.35	0.57
1:B:17:VAL:O	1:B:21:MET:HG3	2.07	0.54
1:A:257:PRO:HG3	4:A:491:HOH:O	2.08	0.53
1:A:298:ARG:NH2	1:B:199:CYS:O	2.42	0.53
1:A:160:GLN:HG3	1:A:239:ARG:HE	1.74	0.53
1:B:17:VAL:HG13	4:B:596:HOH:O	2.09	0.53
1:A:162:VAL:HA	1:A:239:ARG:CG	2.37	0.51
2:C:133:HTI:HAJ2	4:C:536:HOH:O	2.09	0.51
4:A:515:HOH:O	2:C:207:MET:HE1	2.11	0.50
2:C:176:GLN:HE22	2:C:195:ILE:H	1.60	0.49
2:C:161:SER:H	2:C:246:HIS:HD2	1.61	0.49
2:C:322:ALA:HB2	4:C:539:HOH:O	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:138:MET:HG2	1:A:142:LEU:HD22	1.93	0.49
1:A:263:VAL:O	1:A:267:LEU:HG	2.13	0.48
1:A:317:ASN:C	1:A:317:ASN:HD22	2.16	0.48
2:C:317:ASN:ND2	4:C:536:HOH:O	2.44	0.47
1:A:78[B]:GLU:OE1	2:C:213:LYS:HE2	2.15	0.47
2:C:152[A]:GLU:HG3	4:C:557:HOH:O	2.13	0.47
1:B:6:PHE:CE2	1:B:334:VAL:HG13	2.49	0.47
2:C:247:ALA:HB1	2:C:312:TRP:CZ2	2.50	0.47
1:A:240:VAL:HG22	1:A:243:PHE:HB2	1.96	0.46
1:B:267:LEU:HD13	1:B:296:VAL:HG11	1.98	0.46
1:A:258:ILE:HD11	1:A:266:MET:CE	2.46	0.46
1:A:213:LYS:O	1:A:214:GLU:N	2.48	0.46
2:C:97:ASN:HD21	3:C:1:OEG:C2	2.12	0.46
1:A:274:GLU:HG2	1:A:276:PHE:CE1	2.51	0.46
1:B:14:THR:HG21	1:B:43:SER:HB3	1.97	0.45
1:A:317:ASN:ND2	1:A:320:LYS:H	2.14	0.45
2:C:246:HIS:CE1	4:C:536:HOH:O	2.69	0.45
2:C:130:ASN:HD21	2:C:325:ASN:HD22	1.63	0.45
1:A:14:THR:HG21	1:A:43:SER:HB3	1.98	0.45
2:C:164:GLY:HA2	4:C:536:HOH:O	2.17	0.44
1:B:24:VAL:HG11	1:B:324:THR:HA	1.99	0.44
2:C:161:SER:H	2:C:246:HIS:CD2	2.36	0.43
1:B:253:GLU:OE2	1:B:305:HIS:NE2	2.43	0.43
1:A:78[B]:GLU:HG3	2:C:207:MET:SD	2.58	0.43
2:C:250:VAL:HG12	2:C:252:VAL:HG13	2.00	0.43
1:A:27:GLU:HG3	4:A:447:HOH:O	2.17	0.43
1:A:28:ARG:HD3	1:A:331:GLU:OE1	2.19	0.43
2:C:156:VAL:O	2:C:235:PRO:HA	2.20	0.42
1:B:7:ASN:OD1	1:B:33:ASP:HB3	2.19	0.41
1:A:146:TYR:CE1	1:A:231:ILE:HD11	2.54	0.41
1:A:202:GLN:HE21	1:A:202:GLN:HB2	1.62	0.41
1:A:251:HIS:CE1	1:A:302:ASP:OD2	2.66	0.41
1:B:281:PHE:HA	1:B:282:PRO:C	2.41	0.41
2:C:133:HTI:HAH	4:C:539:HOH:O	2.21	0.40
1:B:130:ASN:HA	1:B:131:PRO:HD3	2.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/336 (90%)	299 (98%)	5 (2%)	0	100	100
1	B	296/336 (88%)	290 (98%)	5 (2%)	1 (0%)	50	43
2	C	334/336 (99%)	320 (96%)	14 (4%)	0	100	100
All	All	934/1008 (93%)	909 (97%)	24 (3%)	1 (0%)	59	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	33	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	254/280 (91%)	241 (95%)	13 (5%)	33	25
1	B	255/280 (91%)	250 (98%)	5 (2%)	68	68
2	C	278/279 (100%)	274 (99%)	4 (1%)	78	80
All	All	787/839 (94%)	765 (97%)	22 (3%)	56	53

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	LEU
1	A	167	LYS
1	A	171	ASP
1	A	202	GLN
1	A	239	ARG

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Mol	Chain	Res	Type
1	A	240	VAL
1	A	263	VAL
1	A	295	LEU
1	A	309	ILE
1	A	311	LEU
1	A	317	ASN
1	A	332	LEU
1	A	334	VAL
1	B	68	VAL
1	B	89	GLU
1	B	121	GLU
1	B	300	ARG
1	B	304	SER
2	C	82	LYS
2	C	263	VAL
2	C	296	VAL
2	C	311	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	202	GLN
1	A	251	HIS
1	A	317	ASN
1	B	67	GLN
1	B	97	ASN
1	B	130	ASN
1	B	194	GLN
1	B	325	ASN
2	C	130	ASN
2	C	155	ASN
2	C	176	GLN
2	C	194	GLN
2	C	234	ASN
2	C	246	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HTI	C	133	2	13,13,14	4.86	2 (15%)	14,16,18	2.63	2 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HTI	C	133	2	-	0/12/15/17	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	133	HTI	O-C	16.38	1.22	1.11
2	C	133	HTI	CB-S	-5.44	1.76	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	133	HTI	CB-S-CAH	7.06	109.64	100.65
2	C	133	HTI	C-CA-N	-6.52	107.32	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	OEG	C	1	-	8,8,8	1.32	0	9,9,9	1.91	2 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OEG	C	1	-	-	0/6/6/6	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	OEG	C3-O2-C2	-3.78	106.42	112.79
3	C	1	OEG	O2-C2-C1	3.63	118.84	110.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	306/336 (91%)	0.21	18 (5%)	22 21	18, 31, 47, 65	0
1	B	302/336 (89%)	0.07	13 (4%)	34 33	18, 31, 57, 63	0
2	C	336/336 (100%)	-0.09	9 (2%)	52 52	14, 23, 36, 53	2 (0%)
All	All	944/1008 (93%)	0.06	40 (4%)	35 34	14, 28, 48, 65	2 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	184	TYR	6.2
1	A	291	LYS	5.7
1	B	191	PHE	5.5
1	A	290	GLY	4.3
1	A	170	ILE	4.2
2	C	3	SER	4.0
2	C	185	PRO	3.9
1	B	244	TYR	3.6
1	B	283	THR	3.6
1	B	41	GLU	3.5
2	C	183	GLY	3.4
2	C	186	ALA	3.3
1	A	163	SER	3.2
1	A	169	GLY	3.1
1	A	41	GLU	3.0
1	A	162	VAL	3.0
1	B	276	PHE	2.9
1	A	164	GLY	2.8
1	A	166	GLY	2.8
1	A	123	ARG	2.8
1	A	289	GLY	2.8
1	B	162	VAL	2.7
1	B	271	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	187	GLU	2.4
1	A	242	VAL	2.4
1	B	43	SER	2.4
1	B	269	GLN	2.4
1	A	4	GLN	2.3
1	A	292	ASP	2.2
1	A	304	SER	2.2
1	B	316	ASP	2.2
2	C	159	TYR	2.1
1	A	168	ALA	2.1
2	C	179	LYS	2.1
1	B	188	THR	2.1
2	C	158	THR	2.1
1	B	280	ASP	2.1
1	A	165	ALA	2.1
1	A	171	ASP	2.0
1	B	293	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	HTI	C	133	14/15	0.12	-0.36	17,24,26,26	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	OEG	C	1	9/9	0.18	3.35	40,41,42,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.